

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

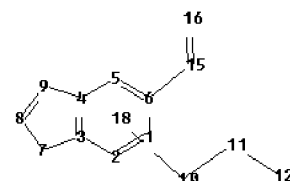
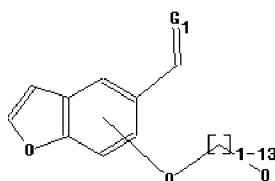
LOGINID:ssptanscl625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

=>

Uploading C:\Program Files\Stnexp\Queries\10507925C.str



```
chain nodes :
10 11 12 15 16
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
6-15 10-11 11-12 15-16
ring bonds :
1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9
exact/norm bonds :
3-7 4-9 7-8 8-9 10-11 11-12 15-16
exact bonds :
6-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
```

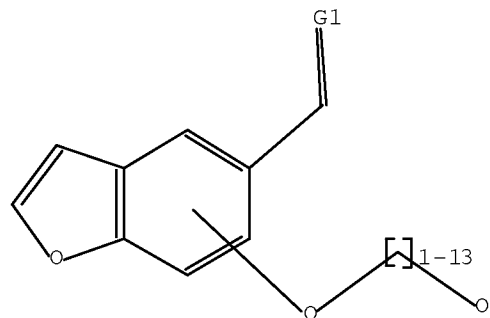
G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atom

L5 STRUCTURE UPLOADED

=> D L5
 L5 HAS NO ANSWERS
 L5 STR



G1 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> S SSS L5 SAM
 SAMPLE SEARCH INITIATED 18:58:39 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 14700 TO ITERATE

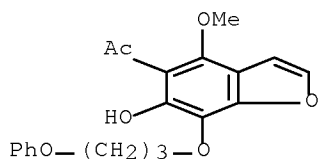
13.6% PROCESSED 2000 ITERATIONS 1 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 286737 TO 301263
 PROJECTED ANSWERS: 1 TO 309

L6 1 SEA SSS SAM L5

=> D SCAN

L6 1 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Ethanone, 1-[6-hydroxy-4-methoxy-7-(3-phenoxypropoxy)-5-benzofuranyl]-
 MF C20 H20 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

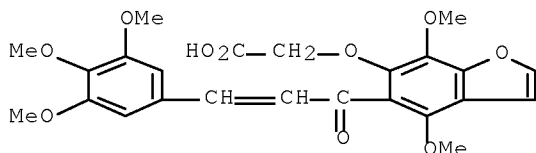
=> S SSS L5 FULL
FULL SEARCH INITIATED 18:58:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 292385 TO ITERATE

100.0% PROCESSED 292385 ITERATIONS 125 ANSWERS
SEARCH TIME: 00.00.02

L7 125 SEA SSS FUL L5

=> D SCAN

L7 125 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Acetic acid, [[4,7-dimethoxy-5-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2-propenyl]-6-benzofuranyl]oxy]- (9CI)
MF C24 H24 O10

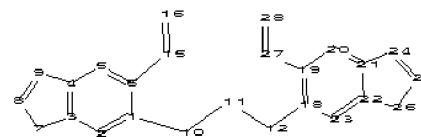
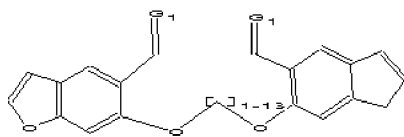


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

.
ENTER NAME OR (END):END

=> SAVE TEMP L7 BAEL10507925/A
ANSWER SET L7 HAS BEEN SAVED AS 'BAEL10507925/A'

=>
Uploading C:\Program Files\Stnexp\Queries\10507925D.str



chain nodes :
10 11 12 15 16 27 28
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26

```

chain bonds :
1-10  6-15  10-11  11-12  12-18  15-16  19-27  27-28
ring bonds :
1-2  1-6  2-3  3-4  3-7  4-5  4-9  5-6  7-8  8-9  18-19  18-23  19-20  20-21  21-22
21-24  22-23  22-26  24-25  25-26
exact/norm bonds :
1-10  3-7  4-9  7-8  8-9  10-11  11-12  12-18  15-16  21-24  22-26  24-25  25-26
27-28
exact bonds :
6-15  19-27
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  18-19  18-23  19-20  20-21  21-22  22-23

```

G1:O,S,N

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:CLASS 28:CLASS

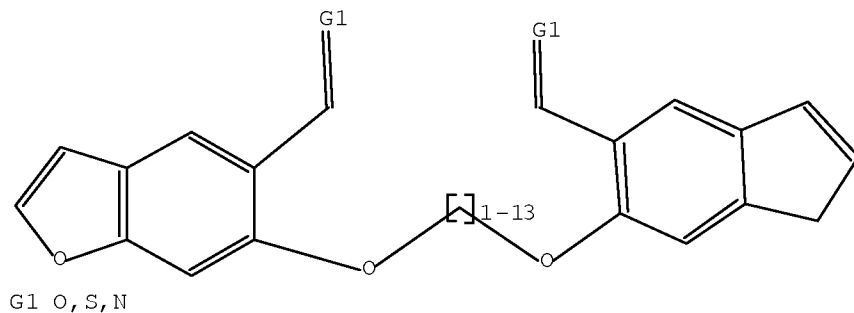
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L8 STRUCTURE UPLOADED

=> D L8

L8 HAS NO ANSWERS

L8 STR



Structure attributes must be viewed using STN Express query preparation.

=> S SSS L8 SAM

SAMPLE SEARCH INITIATED 19:05:47 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 94 TO ITERATE

100.0% PROCESSED 94 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1299 TO 2461

PROJECTED ANSWERS: 0 TO 0

L9 0 SEA SSS SAM L8

=> S SSS L8 SUBSET=L7 SAM

SAMPLE SUBSET SEARCH INITIATED 19:06:23 FILE 'REGISTRY'

SAMPLE SUBSET SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):

ONLINE **COMPLETE**

PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):

0 TO 0

PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):

0 TO 0

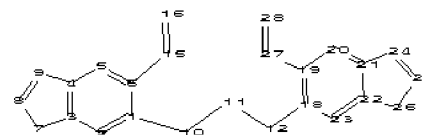
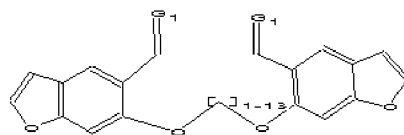
L10 0 SEA SUB=L7 SSS SAM L8

=> D SCAN

L10 HAS NO ANSWERS

=>

Uploading C:\Program Files\Stnexp\Queries\10507925E.str



chain nodes :

10 11 12 15 16 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26

chain bonds :

1-10 6-15 10-11 11-12 12-18 15-16 19-27 27-28

ring bonds :

1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9 18-19 18-23 19-20 20-21 21-22
21-24 22-23 22-26 24-25 25-26

exact/norm bonds :

1-10 3-7 4-9 7-8 8-9 10-11 11-12 12-18 15-16 21-24 22-26 24-25 25-26
27-28

exact bonds :

6-15 19-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom

23:Atom 24:Atom

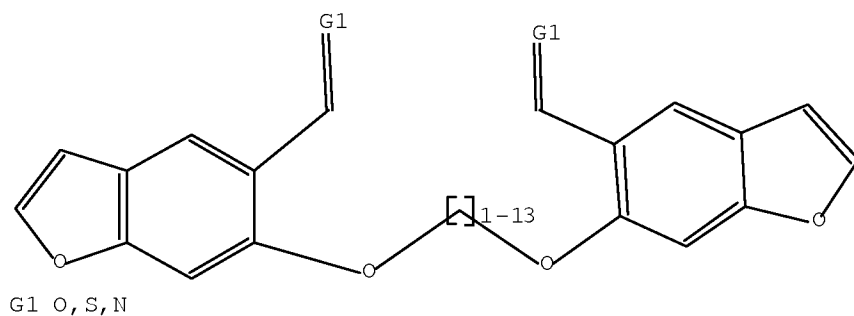
25:Atom 26:Atom 27:CLASS 28:CLASS

L11 STRUCTURE UPLOADED

=> D L11

L11 HAS NO ANSWERS

L11 STR



Structure attributes must be viewed using STN Express query preparation.

=> S SSS L11 SAM

SAMPLE SEARCH INITIATED 19:08:16 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 112 TO ITERATE

100.0% PROCESSED 112 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1606 TO 2874

PROJECTED ANSWERS: 0 TO 0

L12 0 SEA SSS SAM L11

=> D HIS

(FILE 'HOME' ENTERED AT 18:40:49 ON 11 MAR 2008)

FILE 'REGISTRY' ENTERED AT 18:41:03 ON 11 MAR 2008

L1 STRUCTURE UPLOADED

L2 1 S SSS L1 SAM

L3 STRUCTURE UPLOADED

L4 1 S SSS L3 SAM

L5 STRUCTURE UPLOADED

L6 1 S SSS L5 SAM

L7 125 S SSS L5 FULL

SAVE TEMP L7 BAE10507925/A

L8 STRUCTURE UPLOADED

L9 0 S SSS L8 SAM

L10 0 S SSS L8 SAM SUB=L7

=> D IBIB ABS HITSTR 1-4

L15 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:87666 CAPLUS Full-text

DOCUMENT NUMBER: 144:331145

TITLE: A New Class of Blockers of the Voltage-Gated Potassium Channel Kv1.3 via Modification of the 4- or 7-Position of Khellinone

AUTHOR(S): Harvey, Andrew J.; Baell, Jonathan B.; Toovey, Nathan; Homerick, Daniel; Wulff, Heike

CORPORATE SOURCE: The Walter and Eliza Hall Institute, Medical Research Biotechnology Centre, Bundoora, 3086, Australia

SOURCE: Journal of Medicinal Chemistry (2006), 49(4), 1433-1441

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:331145

AB The voltage-gated potassium channel Kv1.3 constitutes an attractive target for the selective suppression of effector memory T cells in autoimmune diseases. We have previously reported the natural product khellinone, as a versatile lead mol. and identified two new classes of Kv1.3 blockers: (i) chalcone derivs. of khellinone, and (ii) khellinone dimers linked through the 6-position. Here we describe the multiple parallel synthesis of a new class of khellinone derivs. selectively alkylated at either the 4- or 7-position via the phenolic OH and show that several chloro, bromo, methoxy, and nitro substituted benzyl derivs. inhibit Kv1.3 with submicromolar potencies. Representative examples of the most potent compds. from each subclass, (5-acetyl-4-(4'-chloro)benzyloxy-6-hydroxy-7-methoxybenzofuran) and (5-acetyl-7-(4'-bromo)benzyloxy-6-hydroxy-4-methoxybenzofuran), block Kv1.3 with EC50 values of 480 and 400 nM, resp. Both compds. exhibit moderate selectivity over other Kv1-family channels and HERG, are not cytotoxic, and suppress human T cell proliferation at low micromolar concns.

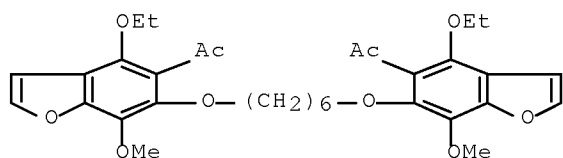
IT 880479-06-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and voltage-gated potassium channel activity of khellinone analogs)

RN 880479-06-1 CAPLUS

CN Ethanone, 1,1'-[1,6-hexanediylbis[oxy(4-ethoxy-7-methoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:446728 CAPLUS Full-text

DOCUMENT NUMBER: 141:251728

TITLE: 1,6-Bis(5-acetyl-4,7-dimethoxybenzofuran-6-yloxy)hexane

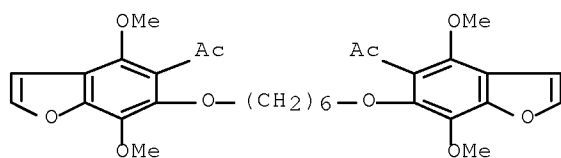
AUTHOR(S): Baell, Jonathan B.; Gable, Robert W.; Harvey, Andrew J.
 CORPORATE SOURCE: Structural Biology Chemistry Group, The Walter and Eliza Hall Institute of Medical Research, Biotechnology Centre, Bundoora, Victoria, 3086, Australia
 SOURCE: Acta Crystallographica, Section E: Structure Reports Online (2004), E60(6), o996-o997
 CODEN: ACSEBH; ISSN: 1600-5368
 PUBLISHER: International Union of Crystallography
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English

AB The khellinone dimer, 1,6-bis-(5-acetyl-4,7-dimethoxybenzofuran-6-yloxy)hexane, C30H34O10, was prepared as part of Kv1.3 ion channel blockers. Crystallog. data are given. The dimer lies on a center of symmetry, and adopts an extended structure such that the separation between the benzofuran groups is 9.927(3) Å. C-H...O H bonds link the mols. into linear chains which lie parallel to the [201] direction.

IT 605665-31-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

RN 605665-31-4 CAPLUS

CN Ethanone, 1,1'-[1,6-hexanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:178993 CAPLUS Full-text

DOCUMENT NUMBER: 140:375004

TITLE: Khellinone Derivatives as Blockers of the Voltage-Gated Potassium Channel Kv1.3: Synthesis and Immunosuppressive Activity

AUTHOR(S): Baell, Jonathan B.; Gable, Robert W.; Harvey, Andrew J.; Toovey, Nathan; Herzog, Tanja; Haensel, Wolfram; Wulff, Heike

CORPORATE SOURCE: Walter and Eliza Hall Institute of Medical Research Biotechnology Centre, Bundoora, 3086, Australia

SOURCE: Journal of Medicinal Chemistry (2004), 47(9), 2326-2336

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:375004

AB The voltage-gated potassium channel Kv1.3 constitutes a promising new target for the treatment of T-cell-mediated autoimmune diseases such as multiple sclerosis. In this study, we report the discovery of two new classes of Kv1.3 blockers based on the naturally occurring compound khellinone, 5-acetyl-4,7-

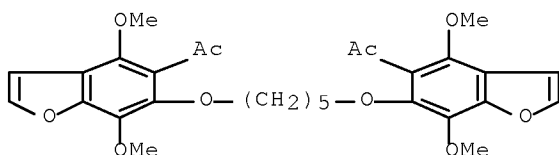
dimethoxy-6-hydroxybenzofuran: (1) khellinone dimers linked via the alkylation of the 6-hydroxy groups and (2) chalcone derivs. of khellinone formed by Claisen-Schmidt condensation of the 5-acetyl group with aryl aldehydes. In particular, the chalcone 3-(4,7-dimethoxy-6-hydroxybenzofuran-5-yl)-1-phenyl-3-oxopropene and several of its derivs. inhibited Kv1.3 with Kd values of 300-800 nM and a Hill coefficient of 2, displayed moderate selectivity over other Kv1-family K⁺ channels, suppressed T-lymphocyte proliferation at submicromolar concns., and showed no signs of acute toxicity in mice. Because of their relatively low mol. weight and lipophilicity and their high affinity to Kv1.3, aryl-substituted khellinone derivs. represent attractive lead compds. for the development of more potent and selective Kv1.3 blocking immunosuppressants.

IT 605665-30-3P 605665-31-4P 605665-32-5P
684278-39-5P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
BIOL (Biological study); PREP (Preparation)
(preparation and immunosuppressive activity of khellinone derivs.)

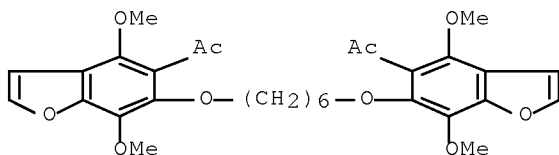
RN 605665-30-3 CAPLUS

CN Ethanone, 1,1'-[1,5-pentanediy]bis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



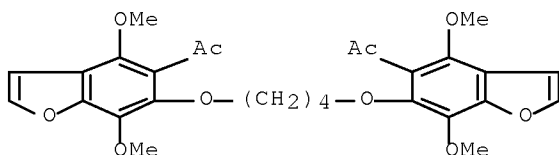
RN 605665-31-4 CAPLUS

CN Ethanone, 1,1'-[1,6-hexanediy]bis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



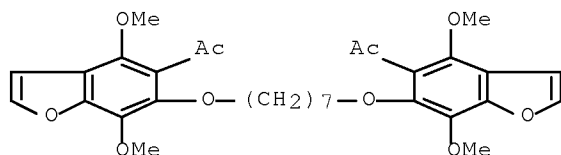
RN 605665-32-5 CAPLUS

CN Ethanone, 1,1'-[1,4-butanediyl]bis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



RN 684278-39-5 CAPLUS

CN Ethanone, 1,1'-[1,7-heptanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



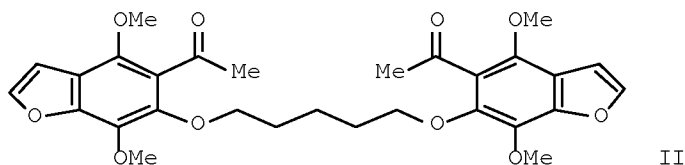
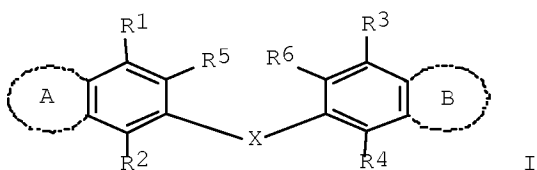
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:757693 CAPLUS Full-text
DOCUMENT NUMBER: 139:276752
TITLE: Preparation of divalent ligands based on khellinone derivatives as therapeutic ion channel blocking agents
INVENTOR(S): Baell, Jonathan B.; Wulff, Heike; Harvey, Andrew J.; Norton, Raymond S.; Chandy, George K.
PATENT ASSIGNEE(S): The Walter and Eliza Hall Institute of Medical Research, Australia
SOURCE: PCT Int. Appl., 64 pp.
 CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003078416	A1	20030925	WO 2003-AU351	20030320
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2479481	A1	20030925	CA 2003-2479481	20030320
AU 2003212101	A1	20030929	AU 2003-212101	20030320
EP 1490349	A1	20041229	EP 2003-707912	20030320
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
CN 1656087	A	20050817	CN 2003-811505	20030320
JP 2005525384	T	20050825	JP 2003-576422	20030320
IN 2004DN02795	A	20070420	IN 2004-DN2795	20040920
US 2005261301	A1	20051124	US 2005-507925	20050705
PRIORITY APPLN. INFO.:			AU 2002-1272	A 20020320
			WO 2003-AU351	W 20030320

OTHER SOURCE(S): MARPAT 139:276752

GI



AB The title compds. [I; R1-R4 = H, OH, alkyl, alkoxy, etc.; X = a divalent spacer group that provides a spacing between the two aromatic rings to which it is joined of from 6 to 11 atoms when measured across the shortest route between the two aromatic rings; A, B = fused rings independently selected from (un)substituted 5-7 membered (hetero)aromatic and non-aromatic heterocyclic rings; R5, R6 = COR7, C(NR7)R7, CSR7 (R7 = H, alkyl, alkoxy, OH); with the proviso] which can be useful in the modulation of potassium channel activity in cells, including among others Kv1.3 channels found in T-cells, were prepared Thus, reacting khellinone with 1,5-dibromopentane in the presence of cesium carbonate in DMF afforded 65% II which showed Kd of 0.82 μ M (Kv1.3) and Kd of 1.5 μ M (Kv1.2). The compds. I may also be useful in the treatment or prevention of autoimmune and inflammatory diseases, including multiple sclerosis. Pharmaceutical composition comprising the compound I was claimed.

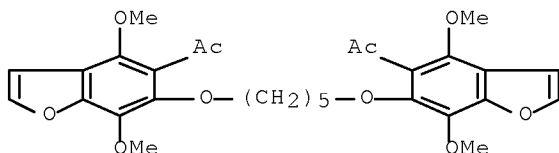
IT 605665-30-3P 605665-31-4P 605665-32-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of divalent ligands based on khellinone derivs. as therapeutic ion channel blocking agents)

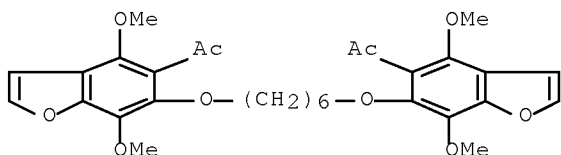
RN 605665-30-3 CAPLUS

CN Ethanone, 1,1'-[1,5-pentanediy]bis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)

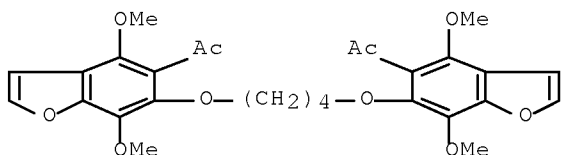


RN 605665-31-4 CAPLUS

CN Ethanone, 1,1'-[1,6-hexanediy]bis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



RN 605665-32-5 CAPLUS
 CN Ethanone, 1,1'-[1,4-butanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> LOGOFF H		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	25.64	267.47
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-3.20	-3.20

SESSION WILL BE HELD FOR 120 MINUTES
 STN INTERNATIONAL SESSION SUSPENDED AT 19:14:06 ON 11 MAR 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptanscl625

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
 SESSION RESUMED IN FILE 'CAPLUS' AT 19:14:46 ON 11 MAR 2008
 FILE 'CAPLUS' ENTERED AT 19:14:46 ON 11 MAR 2008
 COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	25.64	267.47
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

	ENTRY	SESSION
CA SUBSCRIBER PRICE	-3.20	-3.20

=>

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=> LOGOFF Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	26.60	268.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-3.20	-3.20

STN INTERNATIONAL LOGOFF AT 19:16:11 ON 11 MAR 2008